INTEGRATED REACTIVE TRANSPORT MODELLING: CHALLENGES AND OPPORTUNITIES FOR IMPROVED PREDICTION OF DIAGENETIC IMPACT ON RESERVOIR QUALITY

F. Whitaker, A. Al-Helal, T. Gabellone, and G. Griffiths

Department of Earth Sciences,
University of Bristol,
Bristol BS8 1RJ, England
Email: Fiona.Whitaker@bristol.ac.uk

ABSTRACT

Process-based numerical modeling offers the potential to improve our predictive concepts for diagenetic modification of reservoir quality, and to better understand drives for fluid flow and resulting reaction patterns. We explore challenges to improve the accuracy of predictions of diagenesis, including specification of more realistic initial distribution of permeability and effective reactive surface area, and diagenetic changes in this distribution. Additional challenges relate to the need to model at length and time scales appropriate to capture key elements of the system, and to better understand controls on solute transport and reactions. Notwithstanding these constraints, we could make more effective use of existing models, for example by extracting information to characterize simulated diagenetic products and developing more general rules about reactions under given flow systems. Finally, simulations of diagenesis in well-constrained modern and ancient systems are needed in order to demonstrate the utility of process-based modeling to reduce risk in prediction of reservoir quality.

INTRODUCTION

Reactive transport models (RTMs) can improve the predictability of carbonate diagenesis and its effect on reservoir quality by:

1. Integrating experimental, observational, and theoretical knowledge about fluid flow and reactions with data from wells and outcrop analogues;
2. Providing quantitative estimates of rates and distribution of diagenesis and its impact on reservoir quality;
3. Describing diagenetic geobodies and trends which can be used to populate geologic models for reservoir simulation;
4. Providing a platform for developing better conceptual models and hypotheses; and
5. Framing new research questions.

Here, we illustrate the potential offered by RTMs using examples drawn from our recent work on dolomitization, driven by brine reflux and geothermal convection. We then consider a number of challenges that are key to developing more meaningful simulations. These challenges range from more realistic specification of initial rock properties and their alteration by diagenesis, to simulating flow and solute transport in highly heterogeneous media, modeling at appropriate length and time scales with meaningful boundary conditions, and finally improving utility and building confidence in model predictions.

OPPORTUNITIES

RTM simulations can provide insight into the dynamics of diagenesis and the operation of both intrinsic and extrinsic controls. A specific focus of our work is the replacement of limestone by dolomite. Dolomites typically have pore systems and reservoir characteristics that differ fundamentally from those of nearby precursor limestones. In some cases, dolomitization can create excellent reservoir potential, but in others it be responsible for destroying it. In addition to the effect of an increase in porosity due to differences in mineral density, permeability can be radically altered by changes in pore structure, and is also impacted by the effects on compaction and fracturing resulting from the increase in mechanical strength. However, reservoir quality can also be significantly altered by associated diagenetic reactions, ranging from precipitation of pore-occluding dolomite and anhydrite cements by refluxing brines, to calcite dissolution by hydrothermal fluids.

RTMs can provide new insights into the interactions between dolomitization and associated diagenetic reactions, as illustrated by simulations of reflux diagenesis. Carbonate platforms tend to build to sea level, often resulting in an extensive shallow body of sea-water with restricted circulation. Here, evaporative concentration can increase fluid density, generating brines that sink downwards and flow laterally to discharge into adjacent ocean basins. This fluid flow system, termed “reflux,” drives replacement of calcite by dolomite, and the Ca^{2+} released by dolomitization reacts with the high SO_4^{2-} brines, resulting in precipitation of $CaSO_4$ (here assumed to be anhydrite) downstream of the zone of dolomitization (Figure 1, Al-Helal et al., 2012a). This occludes porosity and reduces permeability, focusing fluid flow at increasingly shallow depth. However, once all the calcite has been dolomitized, further reflux dissolves the diagenetic $CaSO_4$ creating a more porous dolomite at shallow depth. It is notable that simulations predict only minor volumes of dolomite cement, in contrast to observations in sequences where “over-dolomitization” has been related to reflux diagenesis (Choquette and Hiatt, 2008).

RTMs also allow us to evaluate the effects of individual controls on a given diagenetic system and target gaps in our knowledge that can provide a focus for future research. These controls can be grouped into factors extrinsic to the system under investigation, such as climate and relative sea-level, and intrinsic controls, such as sediment permeability and reactivity.

A key extrinsic control on reflux diagenesis is climate, which can be constrained for ancient carbonate sequences using paleogeographic reconstructions and paleoclimate models. Solar insolation drives evaporative generation of brines, and also controls the temperature of the platform top. For 85‰ brines, the predicted rate of reflux dolomitization increases with platform top temperature up to 40°C (Figure 2). However, the effect on associated $CaSO_4$ precipitation is even more marked, and at temperatures >40°C, the resulting porosity reduction can limit the vertical extent of dolomitization. This effect is separate from the increase in both fluid density-driven fluid flux and the Mg^{2+}/Ca^{2+} of the brine, which also result from higher rates of evaporation (Al-Helal et al., 2012b).

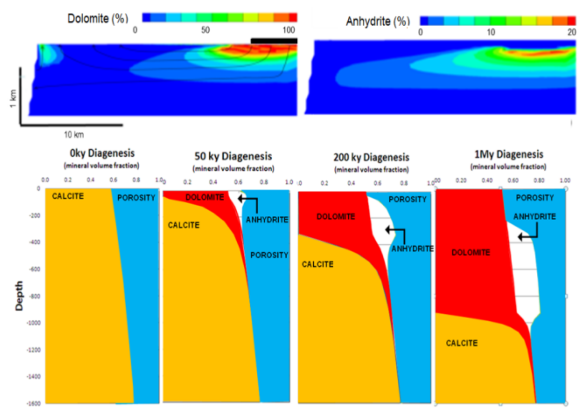

Figure 1. Dolomitization and anhydrite precipitation driven by reflux of 85‰ brines from a 5 km wide pool (black bar) in the center of a broad grain-dominated packstone platform, showing 2D distribution after 1 My of reflux, and 1D evolution over time for a synthetic well in the center of the brine pool.

Intrinsic controls of permeability and effective reactive surface area also play a key role in determining the distribution of diagenetic product formed under a given fluid flow system. The rate of diagenesis increases with both fluid flux and sediment reactivity, but these properties are generally inversely correlated. Fluid flux will be higher in more permeable sediments, which are often the grainier parts of the system, where the reactive surface area may be lower. In contrast, muddier sediments may be less permeable but generally have a much higher reactive surface area. In both cases, differences span several orders of magnitude.

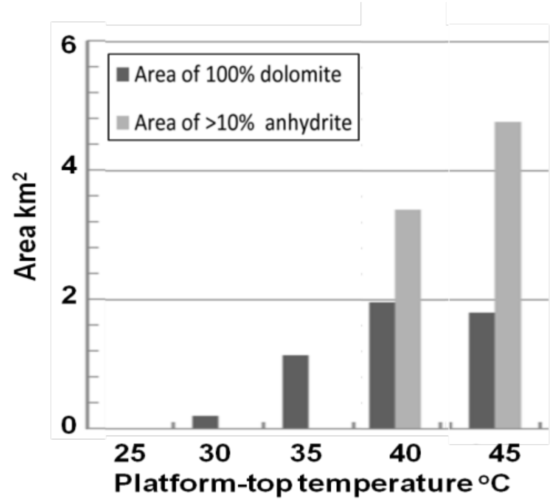

Figure 2. Sensitivity of dolomite and anhydrite abundance formed by reflux of 85‰ brines over 1 My to changing platform top temperature from 40°C of base-case simulation presented in Figure 1.

The relative importance of these two competing intrinsic controls depends upon the Damköhler number (the ratio of the chemical reaction rate to the mass transfer rate). Natural systems will usually comprise a mixture of grainer and muddier sedimentary units. In flow systems where reaction rate limits diagenesis (i.e., high Damköhler number), muddier sediments with higher effective reactive surface area will be altered more rapidly. However, where flow rates are the limiting factor (i.e., low Damköhler number), diagenesis will be more rapid in more permeable, though less reactive, grainier sediments.

This is exemplified by a pair of simulations of dolomitization driven by geothermal convection in the absence of any brine reflux (Figure 3). In contrast to the complex lateral and vertical variations in sediment texture in natural systems, we specify very crude layering. Fifty-meter-thick horizontal beds of either grainstone or mudstone are specified at 200 m depth intervals within the standard grain-dominated packstone platform. Platform groundwater, warmed by geothermal heating, rise buoyantly to discharge at the platform top, and this draws in colder waters from the adjacent ocean basin. Muddy layers within a grain-dominate packstone platform restrict geothermal convection, allowing conduction to warm the interior of the platform. Reactions are flux limited, and dolomitization occurs preferentially in the coarser units near to the platform margin. In contrast, grainstone layers allow convection of cold ocean waters into the platform interior. As a result, reaction rate rather than fluid flux limits dolomitization, which occurs across the whole platform top but is much slower within the grainstone layers.

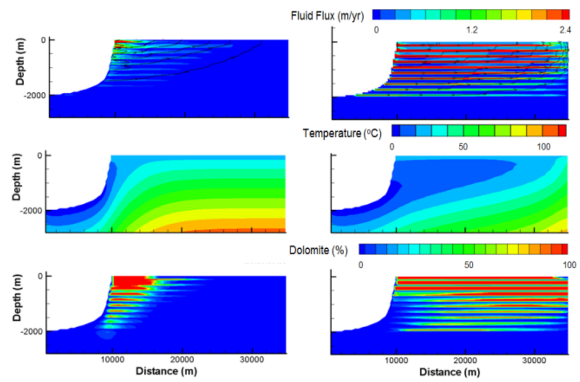

Figure 3. 2D distribution of fluid flux, temperature and dolomitization resulting from geothermal convection in a grain-dominated packstone platform with layers of mudstone (left) and grainstone (right). From Whitaker and Xiao (2010).

CHALLENGES

To better model inherently heterogeneous permeability systems

More realistic representation of spatially variable matrix properties is limited largely by the availability of data describing their distribution in two or three dimensions. Geologic models developed as inputs to reservoir simulation models, and/or forward sediment models, both provide sources of this data. However, appropriate property data may require back-stripping to remove the effect of burial and/or diagenesis post-dating the diagenetic episode of interest. Incorporating more realistic complexity in the initial permeability field results in sharper gradients in diagenetic products reflecting, for example, contrasts in depositional texture. Diagenetic rates are sensitive to the initial mineralogy and the effective reactive surface, which should reflect the nature of the carbonate grains rather than simply their grain size.

RTMs such as TOUGHREACT (Xu et al., 2006) explicitly simulate changes in porosity, and then infer resulting changes in matrix permeability. However simple relationships may fail to represent changes in permeability that can result from textural alteration during diagenesis. For example, the impact of calcite dolomitization on the porosity-permeability relationship is highly variable, dependent upon the type of dolomite. Thus, the Carmen-Kozeny relationship may be adequate for mimetic dolomitization, where grain morphologies are largely unaltered, but poorly represents changes resulting from growth of sucrosic dolomite crystals within a muddy matrix.

Furthermore, the nature and abundance of any associated cements needs careful consideration. A minor amount of vadose cementation at pore throats can give a more significant reduction in permeability than a larger volume of pore-lining phreatic cements. Laboratory measurements and pore-scale numerical experiments allow direct quantification of these effects, and development of more sophisticated algorithms to account for textural changes. In association with this, there is a need to develop our understanding of how dissolution, recrystalization, and cementation affect reactive surface area. Both these effects, operating at scales from the mineral-fluid interface to linked pores, need then to be incorporated into RTMs.

Incorporation of fracture systems and their effect on flow, transport, and reaction remains a major challenge. Neither discrete fracture models or dual permeability models correctly represent fracture-matrix interactions. Geologically more realistic simulations of fracture-matrix interactions (discrete fracture matrix models) are possible (e.g., Belayneh et al., 2006), but at present are more challenging to construct and parameterize.

<u>To model at length and time scales appropriate to capture key elements of the system</u>

Model dimensions need to be appropriate, and only some 3D systems can be meaningfully reduced to 2D. For example 2D simulations of interactions between a discrete fracture and the surrounding matrix will fail to capture the effects of geothermal convection along the plane of the fault (Lopez & Smith, 1995). Coupled with this, discretization of the model domain needs to be at a sufficiently high resolution that the physical processes can be correctly represented (e.g., Yamamoto and Doughty, 2009).

Specification of appropriate boundary conditions is critical for meaningful simulations. One solution is to adopt an embedded approach, in which a larger-scale model is used to condition smaller-scale, but computationally more intensive, simulations. Where reactions of interest occur at relatively shallow depth, they will likely be influenced by boundary conditions that change significantly over the period of diagenesis. The first challenge is then to identify the timescale which controls the system. Thus, for example, in simulating shallow meteoric diagenesis, simple use of a mean annual recharge rate is misleading. In reality, it may be the seasonality of climate, with a switch from net recharge during the wet season to intervening periods of net evapotranspiration, which drives cycling between periods of porosity generation and occlusion (Figure 4). The resulting reorganization of the pore space cannot be derived simply from the total porosity.

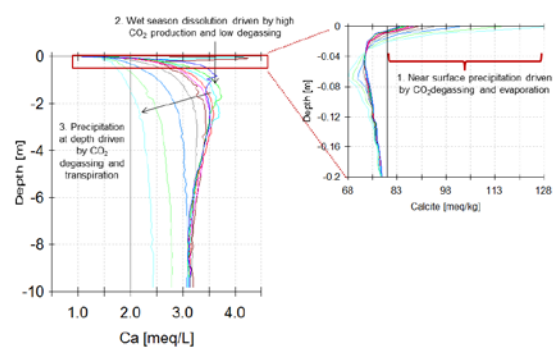

Figure 4. Temporal evolution of calcite dissolution in sands colonised by semi-arid vegetation driven by storms of 100 mm/d recurring at 4-day intervals, followed by 3 dry months of 2 mm/d transpiration (Whitaker and Smart, unpublished research), predicted using HYDRUS (Šimůnek et al., 2008)

More problematic is the simulation of diagenetic processes in areas of rapid sedimentation, which really require explicit coupling between sediment accumulation and changes in boundary conditions governing flow and reactions. While computational limitations currently challenge direct coupling of forward sediment and RTMs, for some problems temporal evolution can be approximated by stepwise addition of active cells and changes in boundary conditions. An alternative approach is to derive simplified rules to predict diagenesis from RTM simulations and build these into forward sediment models, such as CARB3D^{+}, to predict early diagenesis (Figure 5).

Any significant alteration of depositional texture by early diagenesis, is likely to influence the nature and rates of subsequent diagenesis. To fully understand diagenetic evolution, it is therefore necessary to model diagenetic processes from the cradle (early marine mineral stabilization, dissolution, and cementation) to the grave (which in reservoir rocks may be associated with hydrocarbon emplacement). It is a general truism that in moving from the syn-depositional environment to a burial regime, the rates of fluid flow and diagenetic alteration decrease, while the boundary conditions generally become more stable. However, processes such as sedimentary and tectonic compaction can continue into the burial regime and may require deformation of the grid and/or changes in the boundary conditions (Frazer et al., 2012). Again, analysis of the evolution of the sedimentary system through time will require coupling of models, in this case enabling interactions between geomechanics and reactive transport to be simulated.

To better understand controls on solute transport and reactions

RTM predictions are only as good as the understanding of the thermodynamics and kinetics of the fluid-rock system of interest derived from laboratory studies. For many minerals, the controls on reactions in porous media are still far from well understood. In the case of dolomitization, we use a rate constant derived from experiments of Arvidson and Mackenzie (1999) at temperatures >115–196°C, and there is considerable uncertainty in extrapolating this to temperatures <100°C. Reaction rates are often accelerated in the laboratory by increasing the ratio of mineral surface area to reactor volume and/or running experiments far from equilibrium. In contrast, waters in natural systems tend toward equilibrium where uncertainties in rate constants are greatest (Bethke, 2008). Furthermore, whereas most experiments are abiotic, reactions such as dolomite precipitation can be significantly microbially mediated, at least under some circumstances.

We also face a fundamental problem in the degree to which we can predict solute transport. Pore-scale flow models can be used to define effective properties for flow, at least for single-phase fluid. However, dependent upon the degree of fluid-flow channelling, much of the solute can remain trapped in virtually stagnant regions of the pore space, and transport is limited by very slow diffusion (Blunt et al., 2012). A more realistic determination of averaged reaction rates requires consideration of the local fluctuations in concentration and flow path.

To improve utility and build confidence in RTM predictions of diagenesis

There are undoubtedly a number of challenges ahead in generating more meaningful RTMs. Notwithstanding, current RTM technologies offer significant opportunities for improved understanding of diagenesis. One way forward to optimize these opportunities is to generate output that is more directly comparable with observational data and/or more useful in generating reservoir models. For example, in addition to predicting changes in mineral volumes, we can retain information relating to temperature at which diagenetic products are formed and the composition of their parent fluids. Model output can also be interrogated to extract statistics describing diagenetic trends or the geometry and spacing of diagenetic geobodies and their key petrophysical properties, which can be used to populate geological models.

Finally, it is important to develop RTM simulations of well-constrained field examples. For example, we are using a case study of the Mississippian Madison Formation of Wyoming, to investigate interactions between different episodes of early reflux dolomitization and later high-temperature fracture-guided dolomitization, focusing on questions relating to Mg^{2+} massbalance requirements, both in terms of plumbing and fluid chemistry. This will both allow us to test the limits of this technology and demonstrate the potential for improving prediction of diagenetic controls on reservoir quality.

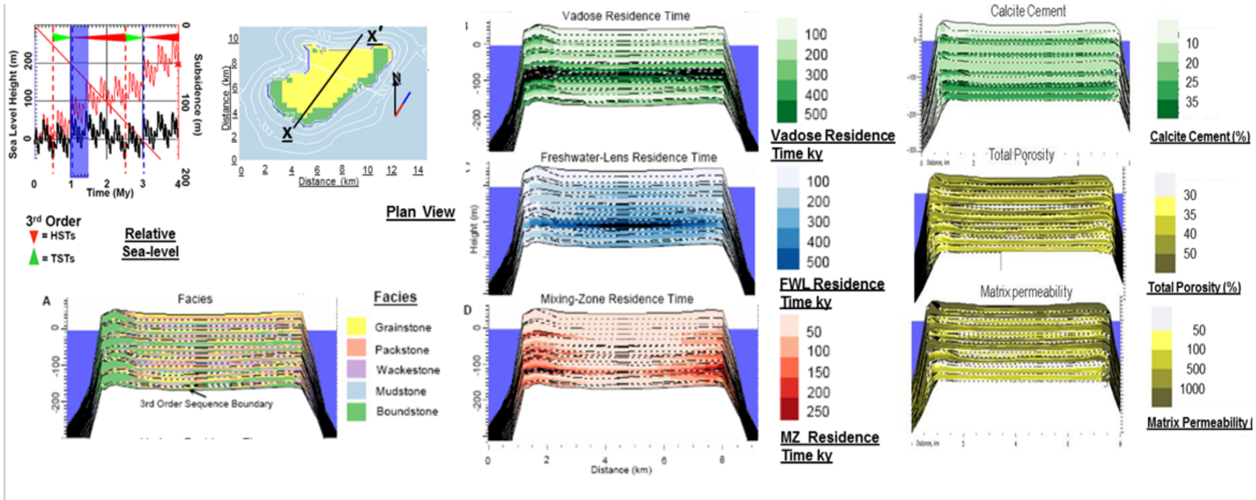

Figure 5. Coupled simulation of architecture, sediment texture, residence time in hydrologically-controlled diagenetic zones (hydrozones) and early diagenesis (calcite cement, porosity and permeability evolution) in a subsiding isolated carbonate platform subject to high-frequency variations in relative sea-level (from study of Paterson et al. (2008) using CARB3D^{+}). Simple diagenetic rules derived from more detailed but essentially static RTM models are used to specify the distribution of diagenesis within these hydrozones.

CONCLUSION

RTMs have the potential to provide a comprehensive, quantitative, and ultimately predictive treatment of diagenetic processes, and their effect on flow behavior and recovery in carbonate reservoirs. They allow simultaneous integration of the major regulatory processes responsible for fluid-rock interaction across a wide range of time and space scales, and can bridge the gap between fundamental, process-oriented research and applied research. However, challenges remain in representation of solute transport and reaction processes, key boundary conditions, and the scale-dependence of key rock properties. While exacerbated by the strong scale dependence in the flow and solute transport of many carbonates, many of these issues also apply to other systems of interest.

ACKNOWLEDGMENT

This research has been supported by sponsors of the Bristol Carbonates Research Group including BG-Group, BHP Billiton, Chevron, ConocoPhillips, ENI, ExxonMobil, Petrobras, SaudiAramco and Wintershall. It has also benefitted from stimulating discussions with many colleagues, including Gareth Jones, Peter Smart and Yitian Xiao.

REFERENCES

Al-Helal, A.B., Whitaker, F.F., Xiao, Y. Reactive transport modelling of brine reflux: dolomitization, anhydrite precipitation, and porosity evolution. *Journal of Sedimentary Research*, 82, 196–215, 2012a.

Al-Helal, A.B., Whitaker, F.F., Spycher, N. Modelling reflux of hypersaline brines using Pitzer ion-interaction model in TOUGHREACT. *Proceedings TOUGH Symposium 2012*, LBNL, Berkeley, California, Sept 17-19, 2012b.

Arvidson, R. S. and Mackenzie, F. T. The dolomite problem: Control of precipitation kinetics by temperature and saturation state. *American Journal of Science*, 299, 257–288, 1999.

Belayneh, M.W. Geiger, S., and Matthäi, S.K. Numerical simulation of water injection into layered fractured carbonate reservoir analogs. *American Association of Petroleum Geologists Bulletin*, 90, 1473-1493, 2006.

Bethke, C.M. *Geochemical and Biogeochemical Reaction Modeling*. Cambridge University Press, 547 pp, 2008.

Blunt, M.J., Branko, B., Gharbi, O. and Mostaghimi, P. From pore structure to mixing and relative permeability in carbonates. *AAPG/SPE/SEG Hedberg Research Conference Fundamental Controls on Flow in Carbonates,* Provence, France, July 8-13, 2012.

Choquette, P.W. and Hiatt, E.E. Shallow-burial dolomite cement: A major component of many ancient sucrosic dolomites. *Sedimentology*, 55, 423-460, 2008.

Frazer, M., Whitaker, F.F., and Hollis, C. Reconstructing Burial Diagenesis in a Post-Rift Regime: The Derbyshire Platform, Northern England. *Proceedings TOUGH Symposium 2012*, LBNL, Berkeley, California, Sept 17-19, 2012.

Lopez D.L. and Smith, L. Fluid Flow in Fault Zones: Analysis of the Interplay of Convective Circulation and Topographically Driven Groundwater Flow. *Water Resources Research*, 31, 1489-1503, 1995.

Paterson, R.J., Whitaker, F.F., Smart, P.L., Jones, G.D. and Oldham, D. Controls on early diagenetic overprinting in icehouse carbonates: Insights from modeling hydrological zone residence times using CARB3D: *Journal of Sedimentary Research*, 78, 258-281, 2008.